Module 1

Impurity atomic species in fusion plasmas, their ionisation state and radiating characteristics

Lecture viewgraphs

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Contents

1.1 Preliminaries

In thermodynamic equilibrium, the radiation field and the distribution functions of particles at a specified temperature, T, are determined from statistical mechanics.

$$u(\tilde{\nu}) = \frac{8\pi h\tilde{\nu}^3}{c^3} / (e^{h\tilde{\nu}/kT} - 1)$$

Planck radiation field energy density

Maxwell speed distribution

$$f(v) = 4\pi \left(\frac{m}{2\pi kT} \right)^{3/2} e^{-\frac{1}{2}mv^2/kT} v^2$$

Boltzmann distribution

$$\frac{N_i}{N_j} = \frac{\omega_i}{\omega_j} e^{(I_i - I_j)/kT}$$

Saha distribution

$$\frac{N_i}{N_+ N_e} = 8 \left(\frac{\pi a_0^2 I_H}{kT} \right)^{3/2} \frac{\omega_i}{2\omega_+} e^{I_i/kT}$$

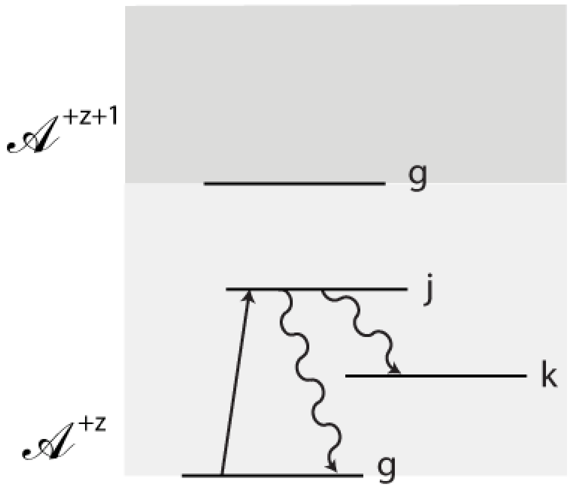
Radiation usually escapes freely from magnetic confinement fusion plasma, so the internal radiation field is zero and populations may be very different from those in thermo-dynamic equilibrium. This enables emission line spectroscopy, but adds complexity to modelling.

1.2 Nomenclature

- For element $\mathscr{A}$, denote the ion charge by *z*, the nuclear charge by z_0 .
  Introduce z_1 = z+1. The number of bound electrons N=z_0-z.
- An iso-electronic sequence is the set of ions with the same number of electrons, such as the Be-like sequence:
  Be^0, B^{+1}, C^{+2}, N^{+3}, ...
- An iso-nuclear sequence, is the set of ions with the same nuclear charge, such as the carbon iso-nuclear sequence:
  C^0, C^{+1}, C^{+2}, C^{+3}, C^{+4}, C^{+5}, C^{+6}
- A spectrum line is specified by giving initial and final states and the wavelength. $\mathrm{CIII}(2s3p\ ^3P \rightarrow 2s3s\ ^3S)\ \ \lambda 464.7\ \mathrm{nm}$
- A spectrum line is really a set of component lines between degenerate groups of initial and final states

configuration	$1s^2 2s3p$	n, l quantum numbers	→	transition array
term	$1s^2 2s3p\ ^3P$	+ S, L quantum numbers	→	multiplet
level	$1s^2 2s2p\ ^3P_1$	+ J quantum number	→	component
state	$1s^2 2s2p\ ^3P_1^{-1}$	+ M quantum number		

2.1 Coronal picture for spectral line emission



Reactions:

$$\mathcal{A}^{+z}(j) \rightarrow \mathcal{A}^{+z}(k) + h\bar{\nu}$$ Spontaneous emission

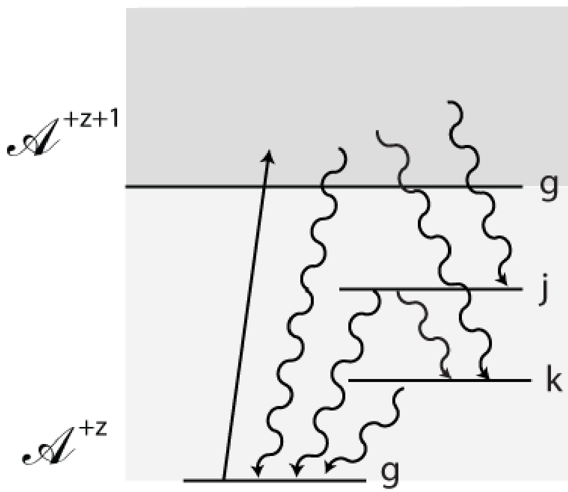
$$\mathcal{A}^{+z}(g) + e \rightarrow \mathcal{A}^{+z}(j) + e$$ Electron impact excitation

Statistical balance: $$N_j = N_e N_g q_{g\rightarrow j}/(A_{j\rightarrow k} + A_{j\rightarrow g})$$

Emissivity: $$\epsilon_{j\rightarrow k} = A_{j\rightarrow k} N_j = N_e N_g A_{j\rightarrow k} q_{g\rightarrow j}/(A_{j\rightarrow k} + A_{j\rightarrow g})$$

Photon emissivity coefficient: $$\mathcal{PEC}_{j\rightarrow k} = A_{j\rightarrow k} q_{g\rightarrow j}/(A_{j\rightarrow k} + A_{j\rightarrow g})$$

2.2 Coronal picture for ionisation



Reactions:

$$\mathcal{A}^{+z+1} + e \rightarrow \mathcal{A}^{+z}(i) + h\tilde{\nu}$$ Radiative recombination

$$\mathcal{A}^{+z}(g) + e \rightarrow \mathcal{A}^{+z+1}(g) + e + e$$ Electron impact ionisation

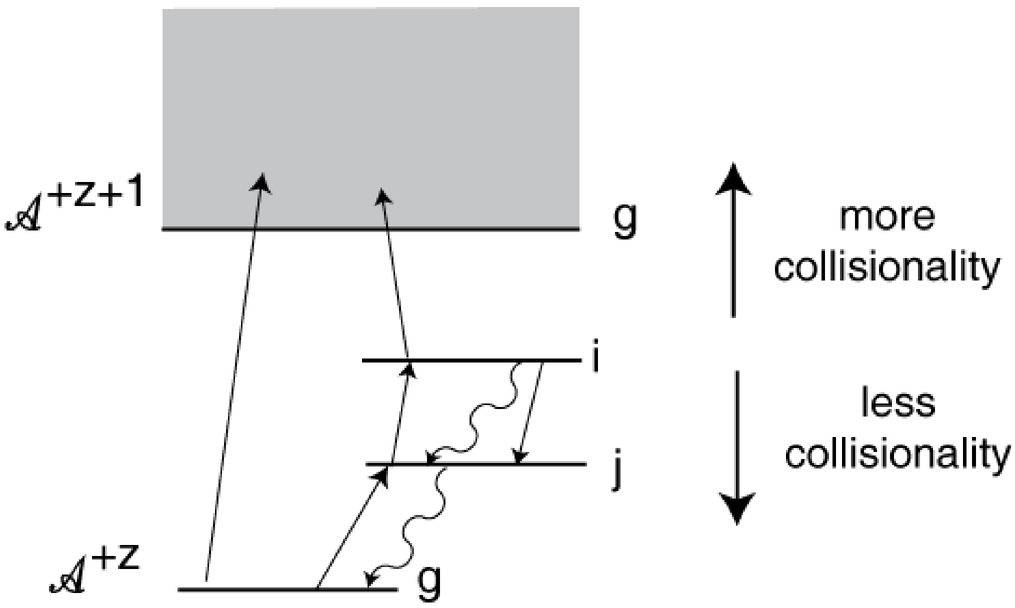
Statistical balance:

$$\begin{aligned}
\alpha_{tot}^{(z+1\rightarrow z)} N_e N^{+z+1}(g) &\equiv (\alpha_j + \alpha_k + \alpha_g) N_e N^{+z+1}(g) \\
&= q_{g\rightarrow\epsilon} N_e N^{+z}(g) \\
&\equiv S_{tot}^{(z\rightarrow z+1)} N_e N^{+z}(g)
\end{aligned}$$

Ionisation balance ratio:

$$\frac{N^{+z+1}(g)}{N^{+z}(g)} = \frac{S_{tot}^{(z\rightarrow z+1)}}{\alpha_{tot}^{(z+1\rightarrow z)}}$$

2.3 Collisional-radiative picture for line emission and ionisation



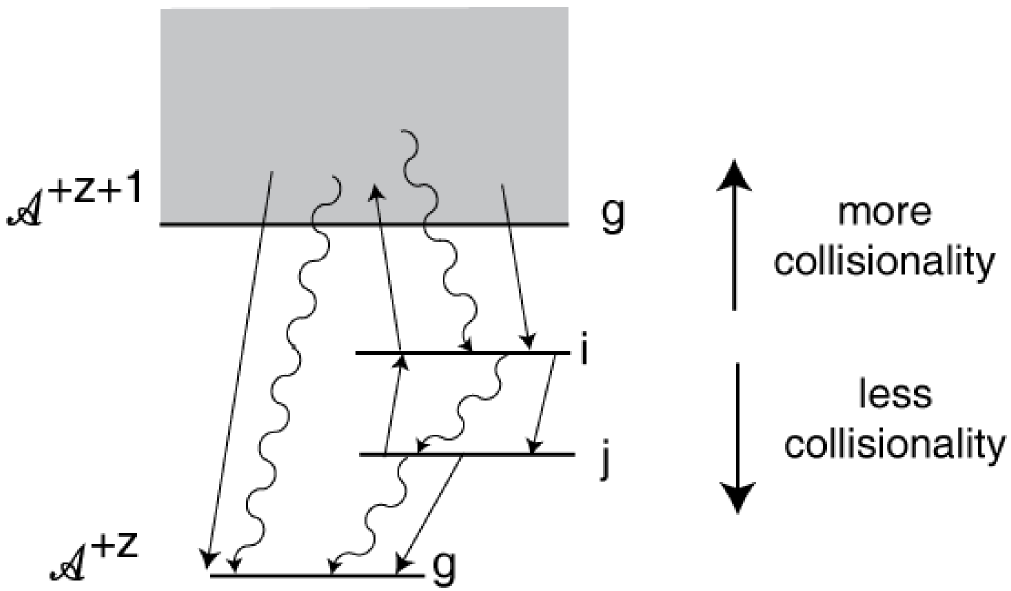
Reactions:

At higher densities, collisional excitation and de-excitation between excited levels compete with spontaneous emission.

$$\mathcal{A}^{+z}(i) + e \rightleftharpoons \mathcal{A}^{+z}(j) + e$$

Indirect pathways lead to line emission and ionisation may occur in a stepwise manner.

2.4 Collisional-radiative picture for line emission and recombination



Reactions:

Three-body recombination must be added to the reactions which pairs with collisional ionisation from excited states

$$\mathcal{A}^{+z}(i) + e \rightleftharpoons \mathcal{A}^{+z+1}(g) + e + e$$

Not all recombinations lead to growth of the ground population of the recombined ion.

2.5 Population equations

In statistical equilibrium:

$$0 = \frac{dN_i}{dt} = \sum_{I_{i'} < I_i} [A_{i' \to i} + N_e q_{i' \to i}] N_{i'} + \sum_{I_{''} > I_i} N_e q_{i'' \to n} N_{i''}$$
$$+ N_e N_+ \alpha_i^{(r)} + N_e N_+ \alpha_i^{(d)} + N_e^2 N_+ \alpha_i^{(3)}$$
$$- \left(\sum_{I_{i''} > I_i} N_e q_{i'' \to i} + \sum_{I_{i'} < I_i} [A_{i' \to i} + N_e q_{i' \to i}] N_{i'} + N_e q_{i \to \epsilon} \right)$$

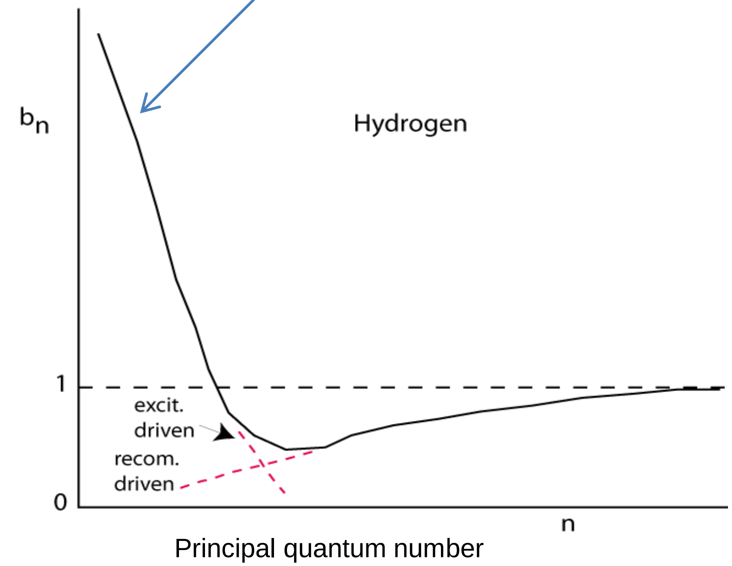
Introduce Saha-Boltzmann deviation factors, b_i

$$\frac{N_i}{N_+ N_e} = \left(\frac{N_i^{(saha)}}{N_+ N_e} \right) b_i = 8 \left(\frac{\pi a_0^2 I_H}{kT_e} \right)^{3/2} \frac{\omega_i}{2\omega_+} e^{I_i/kT_e} b_i$$

Solve for b_i : i=1,...., ∞

Bundle-n model for hydrogen at low density and temperature

T_e ~ 0.5 eV, N_e ~ 10^4 cm^{-3}



Algebraic matrix representation:

$$\sum_j C_{ij} N_j = r_i N e N_1^+ \qquad i = 1, \cdots$$

$$\frac{N_j}{N_e N_1} = \sum_{k, k \neq 1} \bar{C}_{jk}^{-1} \bar{C}_{k1} \left(\frac{1}{N_e} \right) + \sum_{k, k \neq 1} \bar{C}_{jk}^{-1} r_k \left(\frac{N_1^+}{N_1} \right) \qquad j = 2, \cdots$$

Collisional-radiative matrix

3.1 Radiative processes: bound-bound

$$\mathcal{A}^{+z}(i) \rightarrow \mathcal{A}^{+z}(j) + h\tilde{\nu}$$

There are various useful quantities related to the Einstein A-value. The line strength is symmetric between initial and final states.

line strength

$$\omega_i A_{i\rightarrow j} = \frac{1}{6}\frac{\alpha^4 c}{a_0}\left(\frac{h\tilde{\nu}}{I_H}\right)^3 \frac{S_{ij}}{e^2 a_0^2}$$

oscillator strength

$$= \frac{1}{2}\frac{\alpha^4 c}{a_0}\left(\frac{h\tilde{\nu}}{I_H}\right)^2 \omega_j f_{j\rightarrow i}$$

$$\frac{1}{2}\frac{\alpha^4 c}{a_0} = 8.032 \times 10^9 \mathrm{s}^{-1}.$$

The oscillator strength is only applicable to dipole allowed transitions.

$$f_{j\rightarrow i} = f'_{j\rightarrow i} g^I_{ij}$$

bound-bound Gaunt factor

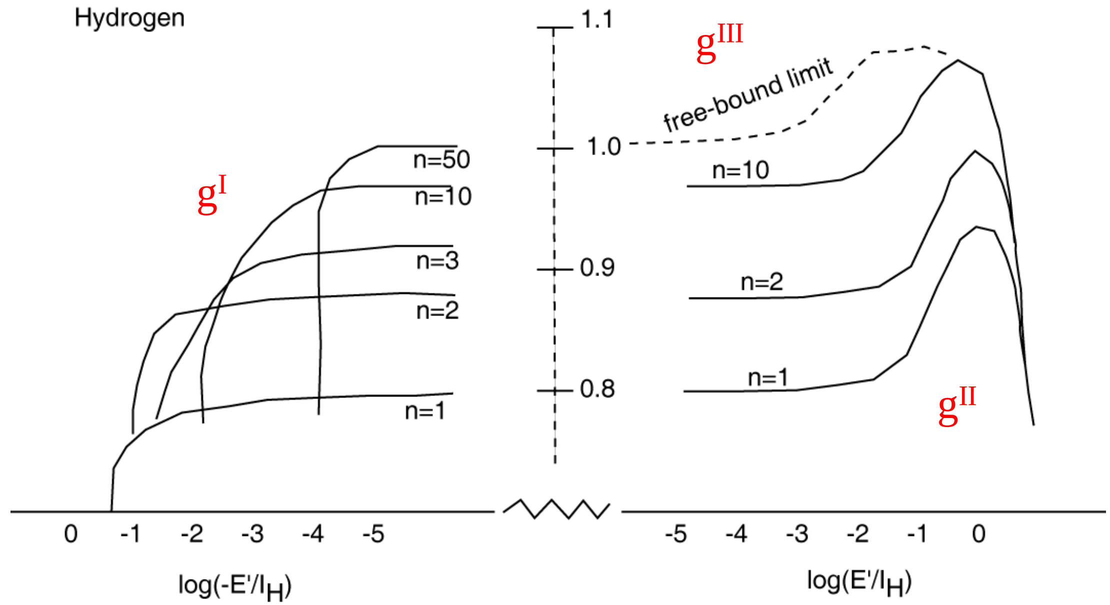
$$A_{i\rightarrow j} = \frac{16\alpha^4 c}{3\sqrt{3}\pi a_0}\frac{1}{\omega_i} z_1^4 \frac{1}{\nu_i^3 \nu_j^3}\frac{1}{\left|\frac{1}{\nu_j^2} - \frac{1}{\nu_i^2}\right|} g^I_{ij}$$

$$\frac{16\alpha^4 c}{3\sqrt{3}\pi a_0} = 1.57456 \times 10^{10}\ \mathrm{s}^{-1}$$

ν_i is the effective principal quantum number for level i. The Gaunt factor is usually fairly close to unity.

3.2 Radiative processes: bound-free

$$\mathcal{A}^{+z+1} + e \rightarrow \mathcal{A}^{+z}(i) + h\tilde{\nu}$$



The Milne relation connects the photo-ionisation cross-section and the capture cross-section

$$Q_c(\tilde{\nu}) = \left(\frac{h\tilde{\nu}}{mvc}\right)^2 \frac{\omega_i}{\omega_+} a(\tilde{\nu})$$

radiative recombination coefficient to level i.

bound-free Gaunt factor

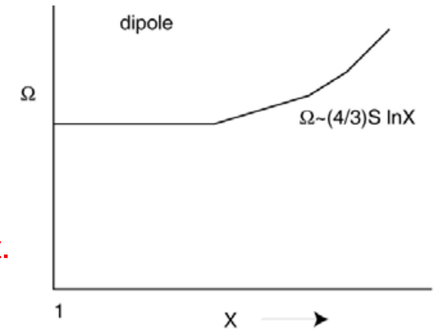
$$\alpha_i(T_e) = 8\left(\frac{\pi a_0^2 I_H}{kT_e}\right)^{3/2} \frac{4\alpha^4 c}{3\sqrt{3}\pi a_0} z_1^4 \left(\frac{2}{\nu_i^3}\right) e^{I_i/kT_e} \int_{I_i/kT_e}^{\infty} \frac{g^{II} e^{-x}}{x} dx$$

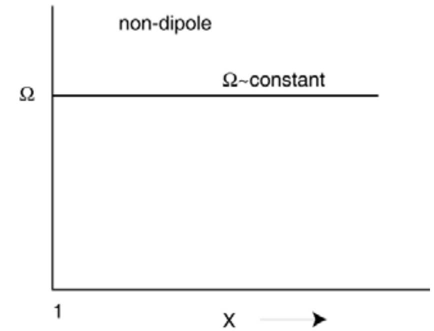
Radiative recombination coefficients are archived in adf08 and prepared by code ADAS211.

3.3 Collisional processes: bound-bound

$$\mathcal{A}^{+z}(i) + e(\epsilon_i) \rightarrow \mathcal{A}^{+z}(j) + e(\epsilon_j)$$

The collisional rate is described by the cross-section. There are useful related quantities.





collision strength

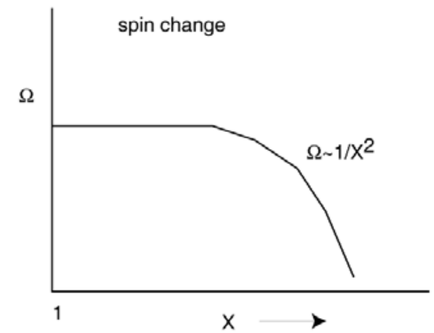
excitation xsect.

de-excitation xsect.

$$\Omega_{ij} = \omega_i \left(\frac{\epsilon_i}{I_H}\right) \frac{\sigma_{i\rightarrow j}(\epsilon_i)}{\pi a_0^2} = \omega_j \left(\frac{\epsilon_j}{I_H}\right) \frac{\sigma_{j\rightarrow i}(\epsilon_j)}{\pi a_0^2}$$

$$\Upsilon_{ij} = \int_0^\infty \Omega_{ij}(\epsilon_j) e^{-\epsilon_j/kT_e} d(\epsilon_j/kT_e)$$

The most useful quantity for tabulation is the Maxwell averaged collision strength



de-excitation rate coefft.

excitation rate coefft.

$$q_{j\rightarrow i}(T_e) = \frac{\omega_i}{\omega_j} e^{\Delta E_{ij}/kT_e} q_{i\rightarrow j}(T_e)$$

Maxwell-averaged collision strength

$$= 2\sqrt{\pi}\alpha c a_0^2 \frac{1}{\omega_i} \left(\frac{I_H}{kT_e}\right)^{1/2} \Upsilon_{ij}(T_e)$$

$$2\sqrt{\pi}\alpha c a_0^2 = 2.1716\times10^{-8} \text{ cm}^3 \text{ s}^{-1}$$

Comprehensive datasets of bound-bound radiative and collisional and energy level data are archived in adf04.

3.4 Collisional processes: bound-free

$$\mathcal{A}^{+z}(i) + e(\epsilon_i) \rightarrow \mathcal{A}^{+z+1}(\rho) + e(\epsilon_\rho) + e(\epsilon'_\rho)$$

$$\mathcal{A}^{+z}(i) + e(\epsilon_i) \rightarrow \mathcal{A}^{+z}(k) + e$$

$$\mathcal{A}^{+z}(k) \rightarrow \mathcal{A}^{+z+1}(\rho) + e$$

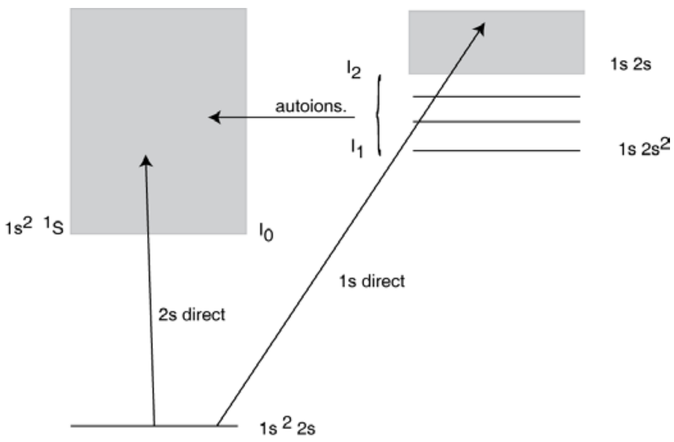
Thompson classical ionisation cross-section

$$\sigma_{i\rightarrow\rho+}(\epsilon_i) = 4\zeta\pi a_o^2\left(\frac{I_H}{I_i}\right)\left(\frac{I_H}{\epsilon_i}\right)\left(1 - \frac{I_H}{\epsilon_i}\right)$$

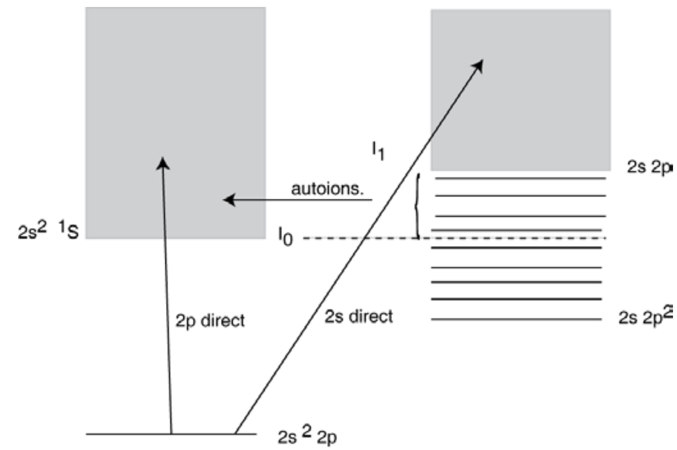
Excitation-autoionisation must be included along with direct ionisation

$$\sigma^{tot}_{i\rightarrow\rho+} = \sigma_{i\rightarrow\rho+} + \sum_k \sigma_{i\rightarrow k}\left(\frac{A_a}{A_a + A_r}\right)$$

$$\sim \sigma_{i\rightarrow\rho+} + \sum_k \sigma_{i\rightarrow k}$$



Li-like ionisation - case(a) example

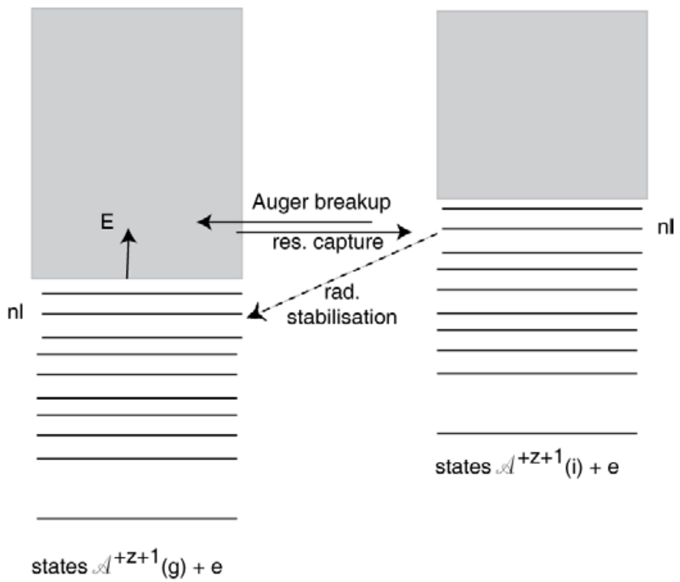


B-like ionisation - case(b) example

$$\sigma^{BCHID}_{tot}(z,\epsilon) = \sum_{i=1}^{m} \sigma^{BCHID}(z, I_i, \zeta_i, \epsilon)$$

ADAS collisional-ionisation data are archived in adf23 and adf07 and prepared offline with ADAS8#2.

3.5 Dielectronic recombination



Reactions:

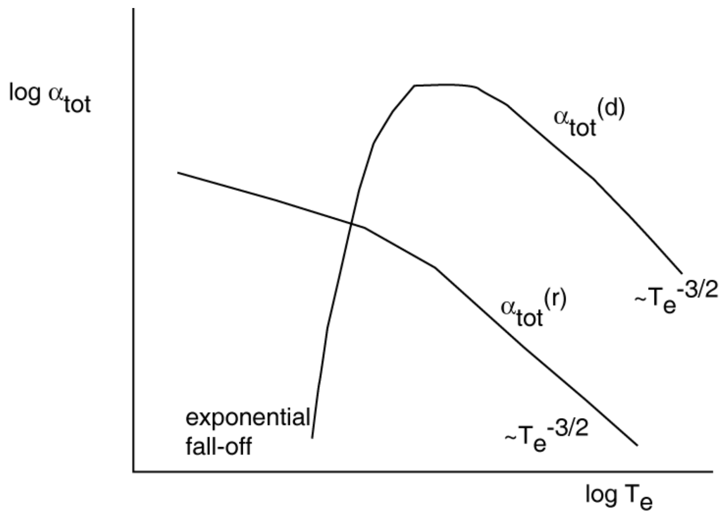
Resonance capture

$$\mathcal{A}^{+z+1}(g) + e \rightleftharpoons \mathcal{A}^{+z}(i, nl)$$

Auger breakup

$$\mathcal{A}^{+z}(i, nl) \rightarrow \mathcal{A}^{+z}(g, nl) + h\tilde{\nu}$$

Radiative stabilisation



Doubly excited populations:

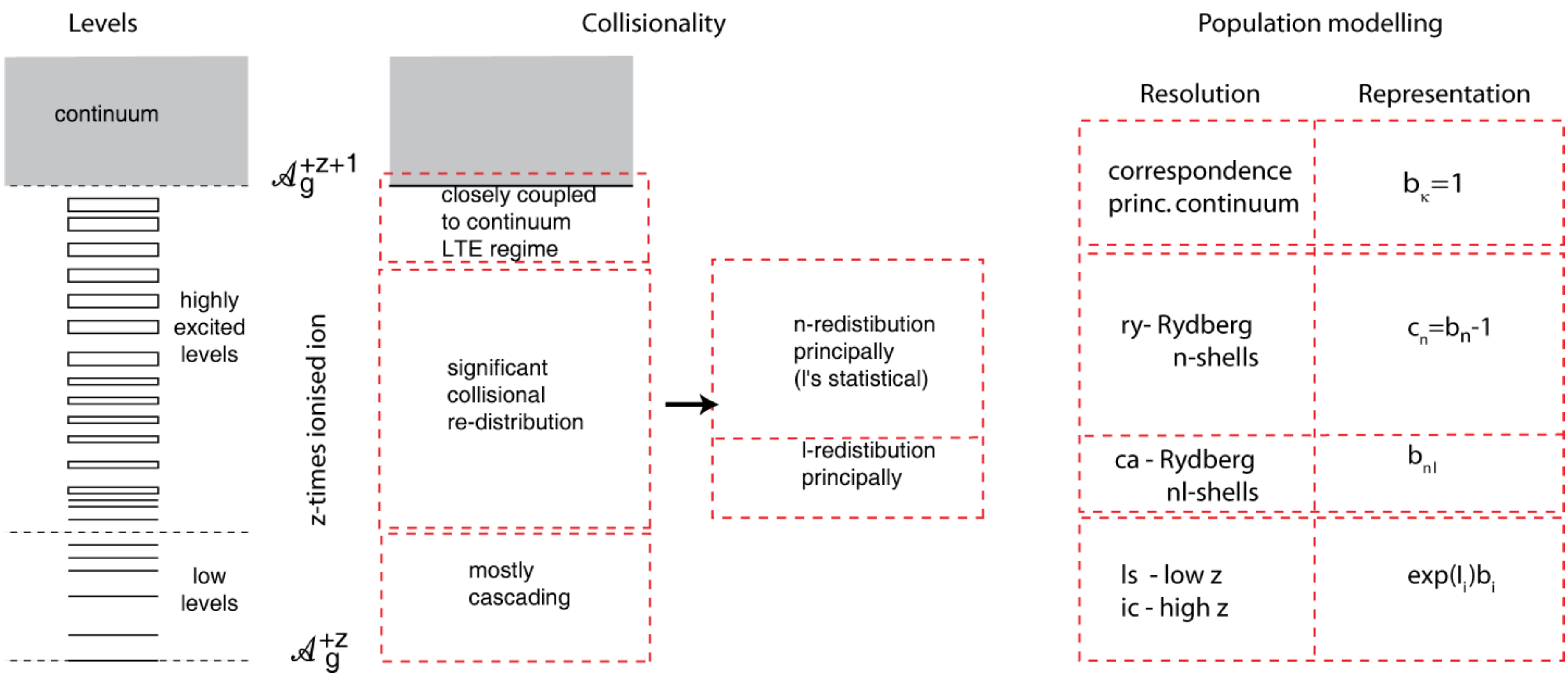
$$b(i, nl) = \frac{A_a}{A_a + A_r}$$

$$\alpha_{tot}^{(d)} = \sum_{i,nl} \alpha^{(d)}(g, i; nl) = \sum_{i,nl} A_r N_{i,nl} / N_e N_g^+$$

At high density there may be re-distribution before stabilisation

State selective dielectronic data are archived in adf09, prepared by Autostructure codes (ADAS series 7)

4.1 Collisionality regimes, grouping and level nomenclatures



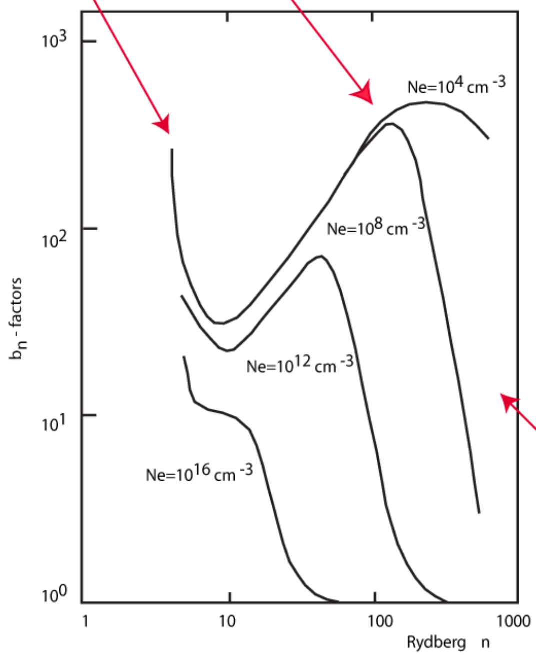
4.2 Bundle-n (*ry*) and bundle-nl (*ca*) populations

b_i - factor defined in term of population $N_i = N_i^{(Saha)} b_i = 8 (\pi a_0^2 I_H/kT_e)^{3/2} (\omega_\iota/2\omega_+) \exp(I_i/kT_e) b_i$

$c_i = b_i - 1$, $expb_i = \exp(I_i/kT_e) b_i$ $\longrightarrow$ b_i , c_i , $expb_i$ representations

$expb_i$ representation required for very low Te

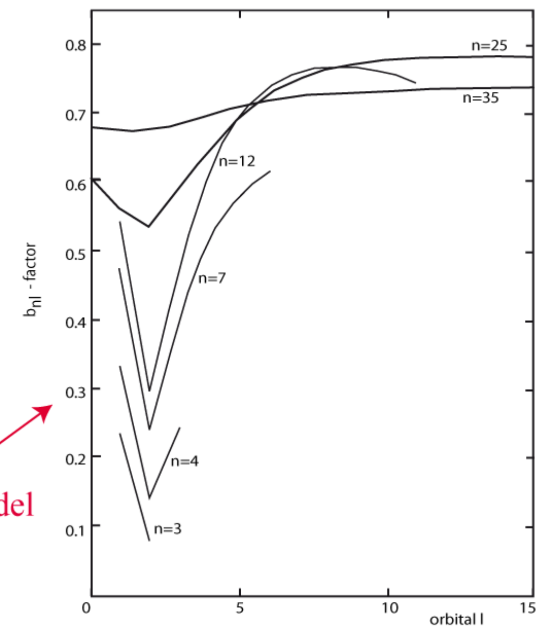
c_i representation required



b_n model

iron population structure Fe^{+14}

b_{nl} model



Hydrogen population structure. Case B depopulated, Ne=10^4 cm^{-3} Te= 1eV

Interactive code ADAS316 is the bundle-n model and ADAS317 is the bundle-nl model

4.3 Low level population structure

Spectroscopy is usually associated with transitions between low lying levels of ions, typically up to the 2nd or 3rd principal quantum shells.

Identify a set of low levels for which all the reactions are available and calculate the population structure for them alone in statistical equilibrium

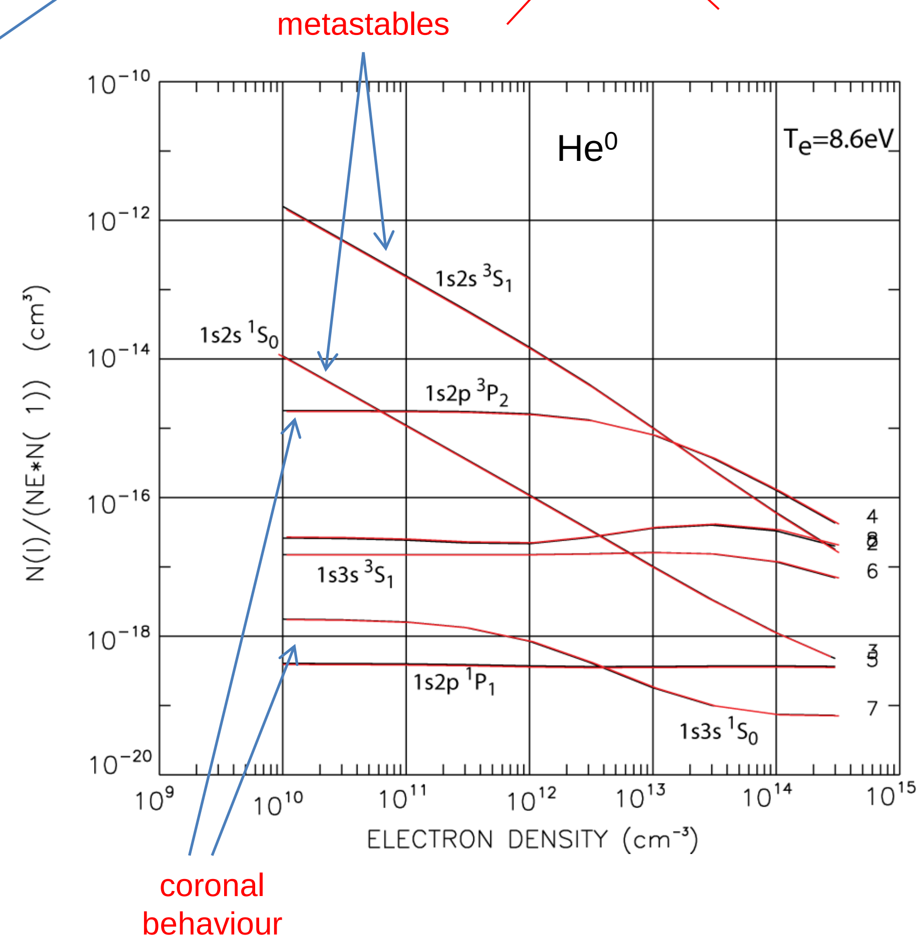
$$\frac{N_j}{N_e N_1} = \sum_{k,k\neq 1} \bar{C}_{jk}^{-1}\bar{C}_{k1}\left(\frac{1}{N_e}\right) + \sum_{k,k\neq 1} \bar{C}_{jk}^{-1} r_k \left(\frac{N_1^+}{N_1}\right) \qquad j = 2, \cdots$$

Some level populations are large (~ N_1) and do not approach coronal behaviour at low densities. These are metastables.

Ordinary excited levels can be treated in quasi-equilibrium with the instantaneous metastable populations. The metastables must be treated as dynamic, in the same manner as the ground states.

Metastables need effective recombination and ionisation coefficients so that their populations can be worked out dynamically in the plasma transport equations.

This is the basis of generalised-collisonal-radiative (*GCR*) modelling.



Interactive code ADAS205 produces the population graphs

4.4 Generalised collisional-radiative picture

Quasi-static assumption and condensation onto metastables

Time dependent population equations take the form below, where focus is restricted to the metastable (indexed by ρ,σ) and ordinary excited (indexed by i,j) populations of $\mathcal{A}^{+z}$.

$$\frac{d}{dt}\begin{bmatrix} N_{\mu}^{+z-1} \\ N_{\rho}^{+z} \\ N_{i}^{+z} \\ N_{\nu}^{+z+1} \end{bmatrix} = \begin{bmatrix} \mathcal{C}_{\mu\mu'} & N_e\mathcal{R}_{\mu\sigma} & 0 & 0 \\ N_e\mathcal{S}_{\rho\mu'} & C_{\rho\sigma} & C_{\rho j} & N_e r_{\rho\nu'} \\ 0 & C_{i\sigma} & C_{ij} & N_e r_{i\nu'} \\ 0 & N_e S_{\nu\sigma} & N_e S_{\nu j} & \mathcal{C}_{\nu\nu'} \end{bmatrix} \begin{bmatrix} N_{\mu'}^{+z-1} \\ N_{\sigma}^{+z} \\ N_{j}^{+z} \\ N_{\nu'}^{+z+1} \end{bmatrix}$$

Make the quasi-static assumption and substitute →

$$\begin{bmatrix} N_{\mu'}^{+z-1} \\ N_{\sigma}^{+z} \\ N_{j}^{+z} \\ N_{\nu'}^{+z+1} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -C_{ji}^{-1}C_{i\rho} & -N_e C_{ji}^{-1} r_{i\nu} \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} N_{\mu}^{+z-1} \\ N_{\rho}^{+z} \\ N_{\nu}^{+z+1} \end{bmatrix}$$

The time-dependence of the metastables is then →

$$\frac{d}{dt}\begin{bmatrix} N_{\mu}^{+z-1} \\ N_{\rho}^{+z} \\ N_{\nu}^{+z+1} \end{bmatrix} = \begin{bmatrix} \mathcal{C}_{\mu\mu'} & N_e\mathcal{R}_{\mu\sigma} & 0 \\ N_e\mathcal{S}_{\rho\mu'} & \mathcal{C}_{\rho\sigma} & N_e\mathcal{R}_{\rho\nu'} \\ 0 & N_e\mathcal{S}_{\nu\sigma} & \mathcal{C}_{\nu\nu'} \end{bmatrix} \begin{bmatrix} N_{\mu'}^{+z-1} \\ N_{\sigma}^{+z} \\ N_{\nu'}^{+z+1} \end{bmatrix}$$

4.5 Generalised collisional-radiative coefficients

Metastable cross-coupling coefficients	$Q^{cd}_{\sigma\to\rho}$	$\equiv \mathcal{C}_{\rho\sigma}/N_e$	$= (C_{\rho\sigma} - C_{\rho j}C^{-1}_{ji}C_{i\sigma})/N_e$	$\mathcal{QCD}$
Effective recombination coefficients	$A^{cd}_{\nu'\to\rho}$	$\equiv \mathcal{R}_{\rho\nu'}$	$= r_{\rho\nu'} - C_{\rho j}C^{-1}_{ji}r_{i\nu'}$	$\mathcal{ACD}$
Effective ionisation coefficients	$S^{cd}_{\sigma\to\nu}$	$\equiv \mathcal{S}_{\nu\sigma}$	$= S_{\nu\sigma} - S_{\nu j}C^{-1}_{ji}C_{i\sigma}.$	$\mathcal{SCD}$

Parent metastable cross-coupling coefficients $X^{cd}_{\nu'\to\nu} \equiv -(S_{\nu j}C^{-1}_{ji}r_{i\nu'})/N_e$ $\mathcal{XCD}$

The photon emissivity coefficients also generalize as:

$$A_{j\to k}N^{+z}_j = \sum_\sigma \mathcal{PEC}^{(exc)}_{\sigma,j\to k}N_eN^{+z}_\sigma + \sum_\nu \mathcal{PEC}^{(rec)}_{\nu,j\to k}N_eN^{+z+1}_\nu$$

excitation recombination

The generalised power coefficients are also obtained

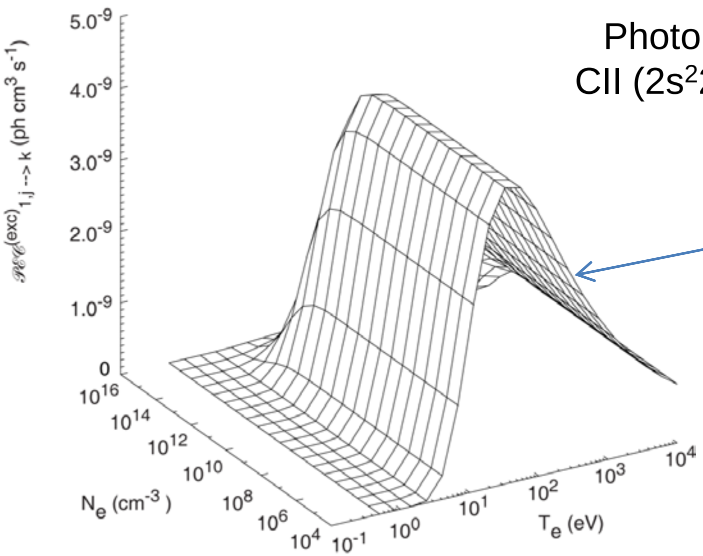
$$\mathcal{PLT}^{(exc)}_\sigma = \sum_{j,k}\Delta E_{jk}\mathcal{PEC}^{(exc)}_{\sigma,j\to k}$$

Low-level line power coefficients

$$\mathcal{PRB}^{(rec)}_\nu$$

Recombination + bremsstrahlung power coefficients

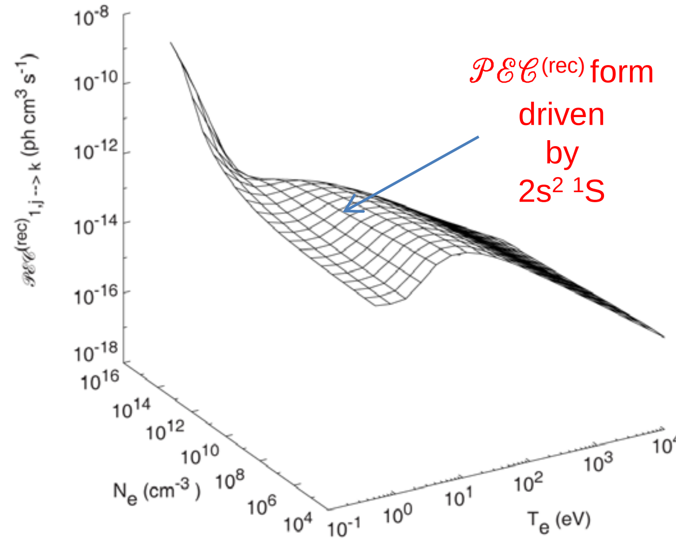
4.6 Coefficient illustrations



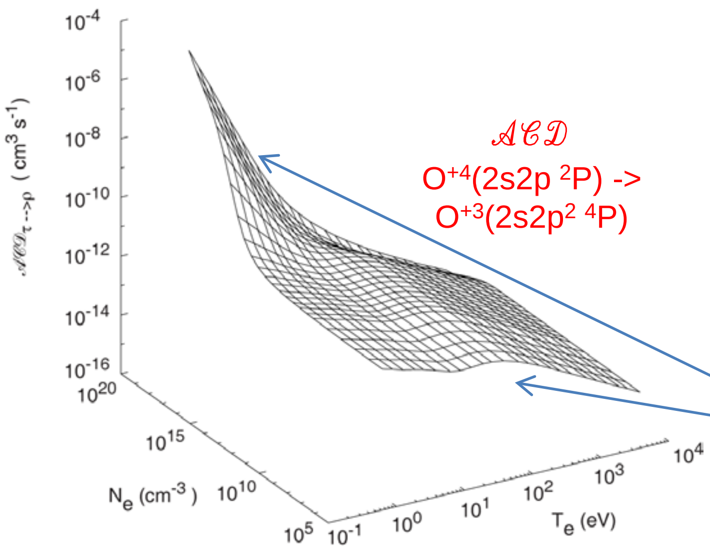
Photon emissivity coefficients
CII ($2s^22p\ ^2P – 2s^23s\ ^2P$) 858.4 A

$\mathcal{PEC}^{(exc)}$ form driven by $2s^22p\ ^2P$

The (exc) form driven by the metastable $2s2p^2\ ^4P$ is ~ factor 10 smaller.

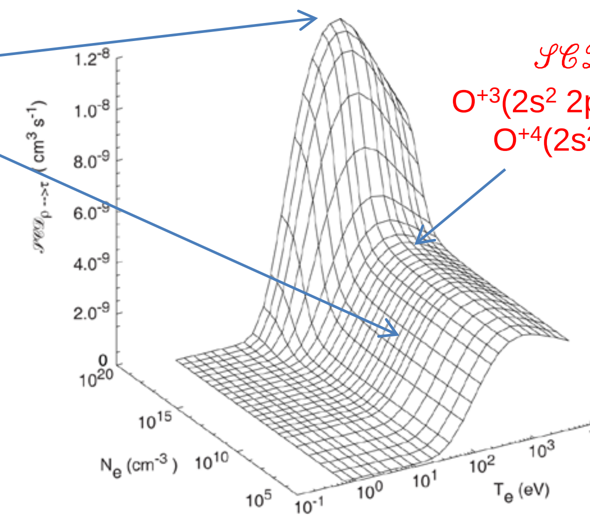


$\mathcal{PEC}^{(rec)}$ form driven by $2s^2\ ^1S$



$\mathcal{ACD}$
$O^{+4}(2s2p\ ^2P) \to O^{+3}(2s2p^2\ ^4P)$

The $\mathcal{SCD}$ coefficient increase to a new limit at high density as excitations lead to ionisation



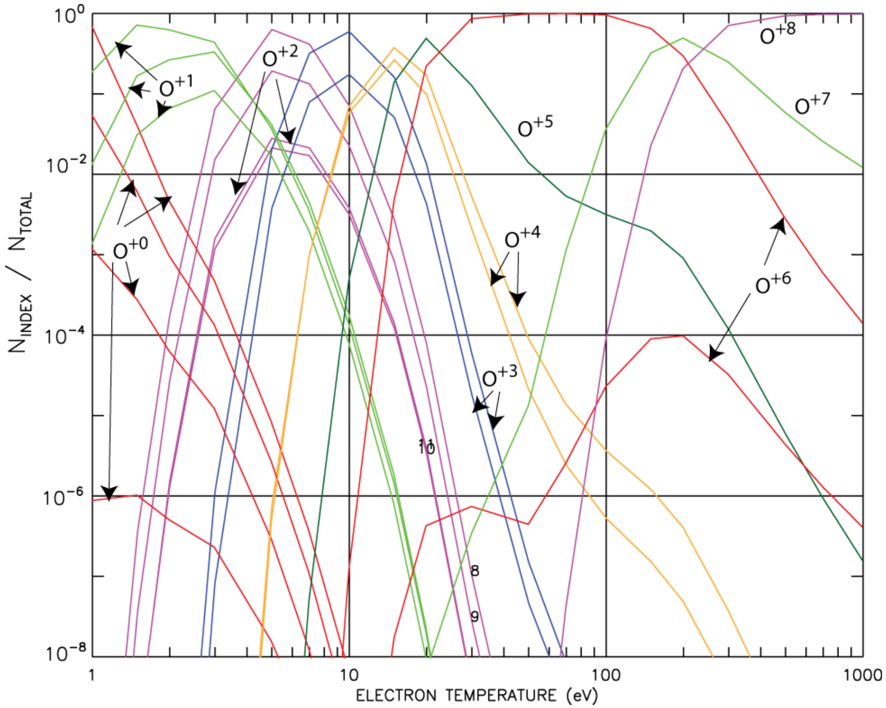
$\mathcal{SCD}$
$O^{+3}(2s^2\ 2p\ ^2P) \to O^{+4}(2s^2\ ^1S)$

The dielectronic part of the $\mathcal{ACD}$ coefficient is suppressed at higher density but rises at low T_e due to three-body recombination

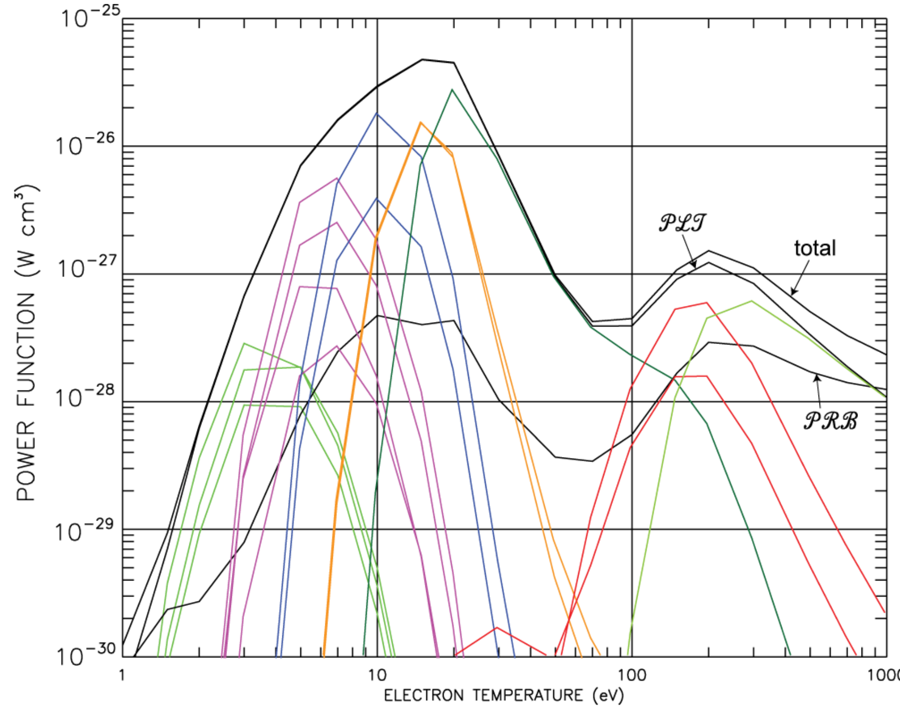
Interactive ADAS208 and offline run_adas208.pro generate the GCR (adf11) , PEC (adf15) and SXB (adf13) data

4.7 Ionisation balance and radiated power

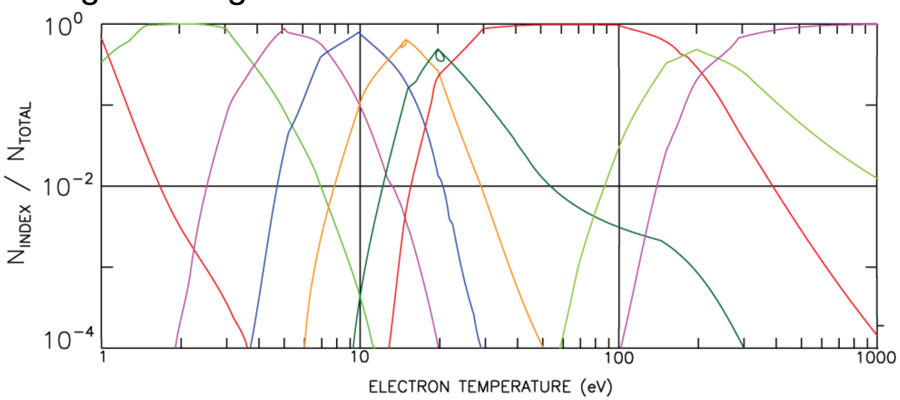
Metastable resolved



Oxygen



Stage-to-stage



Interactive ADAS405 and off-line run_adas405.pro for ionisation balance. A simple transient model is provided by ADAS406 and run_adas406.pro.

Usually GCR and PEC coefficients enter transport codes SANCO, EDGE2D and UTC.

5.1 Conclusions

- This has been rather a race through basic atomic physics of atoms in plasmas. I have made up much more substantial notes for the lecture which are available to participants. I hope these will clarify and expand on points which I have treated cursorily.

- Module 2 builds upon this foundation, seeking to bring population and ionisation state modelling fully up-to-date and particularly addressing the complex issues raised by heavy species such as tungsten in fusion plasma.

- We shall now move on to showing how ADAS is used to calculate the various quantities described here, or at least where to find them and interrogate them in the ADAS databases.

- ADAS has comprehensive CR and GCR data to study all the light elements hydrogen to neon, and silicon. The GCR database will be extended to all elements up to argon in the near future.

- Our decision to number ADAS data formats and codes makes things a little difficult for the newcomer to ADAS. One does get used to these numbers and most people in the international fusion community, working towards ITER, now know what at least adf11 and adf15 data are.

- I draw your attention to the annual ADAS course which follows the ADAS Workshop each year. It is a more leisurely course, of one or two weeks, on ADAS, which some of your colleagues have attended. The notes and tutorial sheets from these courses are available in the ADAS documentation. These may help if our three-day visit is a bit too short to answer all the questions.